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THE BEHAVIOUR OF DETONATION WAVES IN SINGLE PHASE  
HETEROGENEOUS SYSTEMS(U) UNIVERSITY COLL OF WALES  
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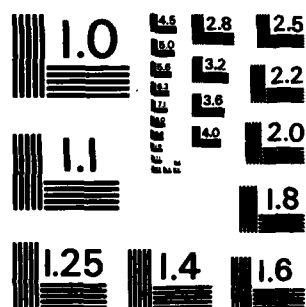
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Grant Number AFOSR-81-0247

THE BEHAVIOUR OF DETONATION WAVES IN SINGLE PHASE HETEROGENEOUS SYSTEMS

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20 November 1982

Interim Scientific Report, No. 1., 30 September 1981 - 29 September 1982

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Prepared for

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and

EUROPEAN OFFICE OF AEROSPACE RESEARCH AND DEVELOPMENT  
London, England.

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## Introduction

Most studies on the ignition and propagation of detonation waves are carried out with systems of uniform composition. However, fuel/air clouds, whether they are produced accidentally or deliberately, will exhibit varying degrees of inhomogeneity. The manner in which both flames and detonation waves propagate in such clouds has received scant attention in the past largely because of the difficulties, both experimental and theoretical, which such problems present. Because of the lack of information on the influence of gradients on wave behaviour it is often tacitly assumed in hazard analyses that the presence of concentration gradients will hamper rather than enhance the propagation of a detonation wave; but this assumption is by no means proven. The present study therefore aims at elucidating the fundamental mechanisms which control the behaviour of detonations in the presence of compositional variations.

Our first involvement with the above problem was some five years ago when Shell Thornton Research Centre were attempting a study of the transmission of a spherical detonation from one volume of gaseous mixture to another which were separated by air gaps of varying thickness<sup>(1)</sup>. It was soon realized that the initial separation of the 'donor' and 'acceptor' gas from the air gap could not be achieved by using stationary membranes, however thin, because they seriously interfered with the gas dynamic processes. It was necessary therefore to explore ways of creating well-defined free surfaces by the removal of rigid slides. During this work the dearth of information on the behaviour of even one-dimensional waves in concentration gradients became apparent. To remedy this serious deficiency in our knowledge, which is of fundamental as well as of immense practical significance, we were awarded an AFOSR grant in September 1981 to pursue this investigation.

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No sooner than this work was started Donato and Lee<sup>(2)</sup> reported some preliminary experiments at the Bordeaux (1981) meeting. Because this work was carried out in a horizontal detonation tube we have been able to show that serious distortions would have occurred in the interfaces and consequently large uncertainties in the experimental data. Recently Topchian<sup>(3)</sup> has reported some work on the transmission of a detonation through an inert gas lock in a tube in order to define the quenching length required. This work, although interesting, is only of marginal relevance to the general problem. The only other fundamental work known to the authors is that of Strehlow and Stiles<sup>(4)</sup> who were the first to study the changes in structural behaviour of a detonation in its transmission from one detonable system to another.

The primary objective of the present work is to study, firstly, in a detonation tube, the interaction of a detonation wave with both abrupt and gradual changes in the concentrations of fuel in air. When these phenomena are better understood the work will be extended to examine the behaviour of a detonation propagating through two concentration gradients at varying separation. The final goal of the study is to elucidate the effect of these wave interactions on the detonability of both partially and totally unconfined fuel/air clouds.

### Experimental

Before meaningful results can be obtained it is essential to be able to create well-defined concentration gradients in the systems under study. Preliminary experiments showed that in a horizontal detonation tube a free interface created by the rapid removal of a thin diaphragm remains reasonably planar for less than one second. Consequently horizontal tubes can only be used for the study of abrupt gradients in which the tube is fired within a fraction of a second following the removal of the diaphragm. In all our work therefore a vertical tube was used as depicted in figure 1. This tube, of internal wall 2.5 x 1.3 cm., is comprised of three sections:

a driver section AB which is used to generate a stable detonation in the donor gas BC, and an acceptor section CD. A stable free interface can be created between donor and acceptor gases by removing slide S.

In order to check on the quality of the diffusional gradients set up by the system a separate section was built to study the density profiles using a Mach-Zehnder interferometer. The agreement between the calculated and observed gradients, shown in figure 2, is very gratifying. The only effect which the removal of the diaphragm seems to have is to produce a rapid oscillation of the interface, with a period of about 0.5 sec, which seems to disturb a thickness of gas of about 5 mm on either side of the interface.

Piezoelectric pressure transducers are mounted in the tube wall to record the pressure profiles and the position of the reaction zones are located by means of ionization probes. In addition, 3 cm wavelength microwaves are launched by an aerial placed in the end wall of the acceptor section. When these are reflected by the ionized burned gases the reflected signal is recorded by the launching aerial and the recorded interference pattern enables the velocity of the reflecting surface to be found. This method has proved extremely useful in monitoring reaction zones over long lengths of tube<sup>(5)</sup>.

A window section W is available for taking both spark and streak Schlieren photographs. Unfortunately the closest edge of the window is 7 cm from the interface so that it is not possible to observe the interactions occurring at the interface itself. Attempts have been made to displace the interface down into the window section; so far, however, the technique has not been successful.

In addition to the window section a smoked-oil section is also available for observation both up-stream and down-stream of the slide valve.

### Planar Interface Studies

In the first series of experiments the interaction of a detonation in  $C_2H_2 + 2.5O_2$  with a steep interface with several inert gases was investigated. Hitherto simple theoretical models, such as that due to Paterson<sup>(6)</sup>, have been used to determine the interaction. In these models the detonation is assumed to behave as a non-reactive shock with a peak pressure equal to the CJ value in the detonation wave. A comparison of the measured velocities of the transmitted shock and the calculated values is given in Table I. It is seen that the agreement is poor, which is not altogether surprising in view of the idealization of the model. Since this work was completed the authors have been informed by Professor Glass<sup>(7)</sup> that an exact numerical calculation which allows for the penetration of the Taylor expansion wave into the flow-field of the transmitted wave, is now available. The application of this analysis to the present results is being undertaken at present.

Table I

Transmitted shock velocities for  $C_2H_2 + 2.5O_2$  | inert gas  
at  $p_0 = 300$  Torr

| Acceptor gas    | Velocity $ms^{-1}$ |                                  |
|-----------------|--------------------|----------------------------------|
|                 | Predicted          | Average measured ( $\sim 20$ cm) |
| He              | 3223               | 2000                             |
| Air             | 1640               | 1270                             |
| Ar              | 1613               | 1200                             |
| SF <sub>6</sub> | 854                | 670                              |
| CO <sub>2</sub> | 1350               | 850                              |

One of the notable features of the pressure profile of the transmitted shock wave is that, in some inert gases, it exhibited a secondary shock wave. Thus in the five inert gases that were studied Air,  $\text{SF}_6$  and  $\text{CO}_2$  the secondary shock was strong whereas in Ar it was relatively weak and in He it was non-existent. An example of the pressure profiles in  $\text{SF}_6$  at different distances from the slide is given in Figure 3. In this particular case the secondary shock grows in strength up to a distance of 20 cm and thereafter decays as it recedes from the main shock front. Schlieren photographs show that it corresponds to a near planar shock wave lying between the shock front and the burned gases, rather close to the latter in fact. Another example of the formation of the secondary shock, this time in  $\text{CO}_2$ , is shown in Figure 4. This clearly shows that it is a phenomenon that occurs when the shock front decouples from the reaction zone. A possible mechanism for the formation of the secondary shock is discussed in the final section of the Report.

#### Studies with concentration gradients

##### (a) Velocity measurement

A series of measurements were made on the velocity of a detonation as it travelled along a concentration gradient in order to see how rapidly the wave velocity adjusted to the local conditions. As in all the experiments of this series  $\text{C}_2\text{H}_2 + 2.5\text{O}_2$  was the donor and the inert diluent was Argon. Concentration gradients of various steepness were created by allowing different diffusion times after opening the slide valve, and the wave velocities were determined by means of the microwave interferometer.

The velocity-distance plots obtained in this manner are given in Figure 5. The upper solid curve in each case is the predicted CJ velocity corresponding to the dilution at a given point which in turn is derived from the diffusion profile. These results are also plotted in Figure 6 in a different way: the velocity at a given



point is plotted as a function of the dilution at that point due to diffusion. The progressive discrepancy between the measured and calculated velocities is due to the increasing influence with dilution of the wall boundary-layer which gives rise to a velocity deficit. This was confirmed by measuring steady-state velocities in the tube at several values of argon dilution. These results are seen to agree closely with the non-steady diffusional cases. Although velocity is not a sensitive parameter to departures from a CJ wave the excellent agreement that is observed gives some support to the view that the detonation adjusts fairly rapidly to the local concentration conditions obtaining in the medium.

(b) Smoked foil records

A far more sensitive test than velocity of the rate of equilibration of a wave is a measure of the cell sizes as provided by a smoked foil placed on the inner surface of the tube wall. A special section with removable plates allowed Mylar foils, coated with a thin layer of soot, to be placed flush with the broad tube wall at distances of 120 - 180 mm and 300 - 560 mm from the interface. The change in transverse wave structure could then be found as a function of distance from the interface for various diffusion times. An example of the results obtained with  $\text{CO}_2$  as a diluent is given in Figure 6. Although there is a large scatter in the measured cell sizes the broad agreement between the steady state detonation values and those for the non-steady propagation lends support to the view that adjustment of the wave to the localized values occurs within a few cell lengths.

(c) Pressure records

We have already observed that the main feature of the pressure records that were obtained with a planar interface was the development of a secondary shock front. However, when a diffusional gradient is allowed to develop then the nature of the record changes markedly

and large amplitude oscillations, corresponding to the fundamental spin mode of the tube, appear as the shock front and the reaction zone decouple. A series of pressure records relating to the oxyacetylene/air system is given in Figure 7. On the same diagram (x, t) plots of both the shock front and the reaction zone are given for a diffusion time of 6 minutes after opening of the slide valve.

One further interesting series of pressure records is shown in Figure 8 which shows the profiles in argon and air gradients both for different diffusion times and different positions from the slide. On the same diagram a pressure record for uniform composition and no dilution is shown as a control, and on each record the calculated CJ pressure level is indicated. Because of the presence of transverse wave oscillations it is difficult to assess the average pressure levels. Nevertheless there is no evidence that the average pressure exceeds the calculated CJ value in any of the records. Consequently no overdriving of the wave is apparent which again confirms the evidence of velocity and cell size observations.

#### Experiments with two concentration gradients

Some preliminary experiments have been carried out in which two slide valves, at various separations, have been employed to generate two concentration gradients. The donor and acceptor systems were  $C_2H_2 + 2.5O_2$  and  $C_2H_2 + 2.5O_2 + 7N_2$  respectively and the inert gas separating them was air. The initial findings show that when the wave in the donor gradient reaches the point of roughly 80% dilution decoupling occurs and the transmitted shock cannot cause direct ignition of the acceptor gas. In general we find that if the donor and acceptor diffusion gradients do not to some degree overlap then instantaneous ignition in the acceptor seldom occurs. In other words, any inert gap whose length exceeds one or two cell lengths is sufficient to cause decoupling of the shock and reaction zone and consequently it fails to cause *direct* initiation in the acceptor

system. Of course ignition occurs in the acceptor at a later stage in most cases through the usual flame transition processes which are well known. However these are not of immediate relevance to the present investigation. There is some indication that the nature of the secondary shock wave and also the amplitude of the transverse waves in the transmitted wave front do exert some influence on the direct initiation of the acceptor but this has not yet been quantitatively evaluated.

### Conclusions

1. When a detonation wave is transmitted through a steep concentration gradient a secondary shock wave is formed which propagates between the transmitted shock and the burned gases. The intensity of this shock depends on the rate of quenching of the detonation which, in turn, depends on the concentration gradient and the heat capacity of the diluent gas. Thus when argon, air,  $\text{CO}_2$  and  $\text{SF}_6$  are used consecutively as diluent gas the strength of the secondary shock progressively increases. The ratio of the acoustic impedances of these gases to that of the detonating system may also be a factor to be considered.

A possible model for the development of the secondary shock is given in Figure 9. This is only a qualitative description and further work, both theoretical and experimental is necessary to establish its applicability to the wave interaction.

2. When the concentration gradient between the reactive and inert gases is less severe, i.e. after some time has elapsed following the removal of the diaphragm, strong transverse waves appear on the pressure records as decoupling occurs between the shock and reaction zone. This is reminiscent of the amplification of transverse waves that occurs in marginal waves.

3. Velocity, pressure and cell size measurement indicate that when a detonation travels in a gradient with one diluent the wave rapidly adjusts to the local CJ values. It must be admitted that this conclusion may be strictly applicable only to the present detonation tube and the reactive system studied. This is because large wall boundary layer losses cause the Taylor expansion wave to be enhanced. It cannot therefore be claimed that the present result is universally true and further work on this problem is required particularly in larger diameter tubes and with gases at a higher initial pressure.

4. Preliminary work using two slide valves to create two variable concentration gradients has given promising results. They show that there are critical concentration gradients, which are characteristic of a given chemical system, for which a detonation will transmit from one system to another without going through the intervening process of flame to shock transition. After some further work with this particular experimental set-up the foundation will have been laid for the extension of the study of the propagation of detonations on three-dimensional gradients in unconfined systems.

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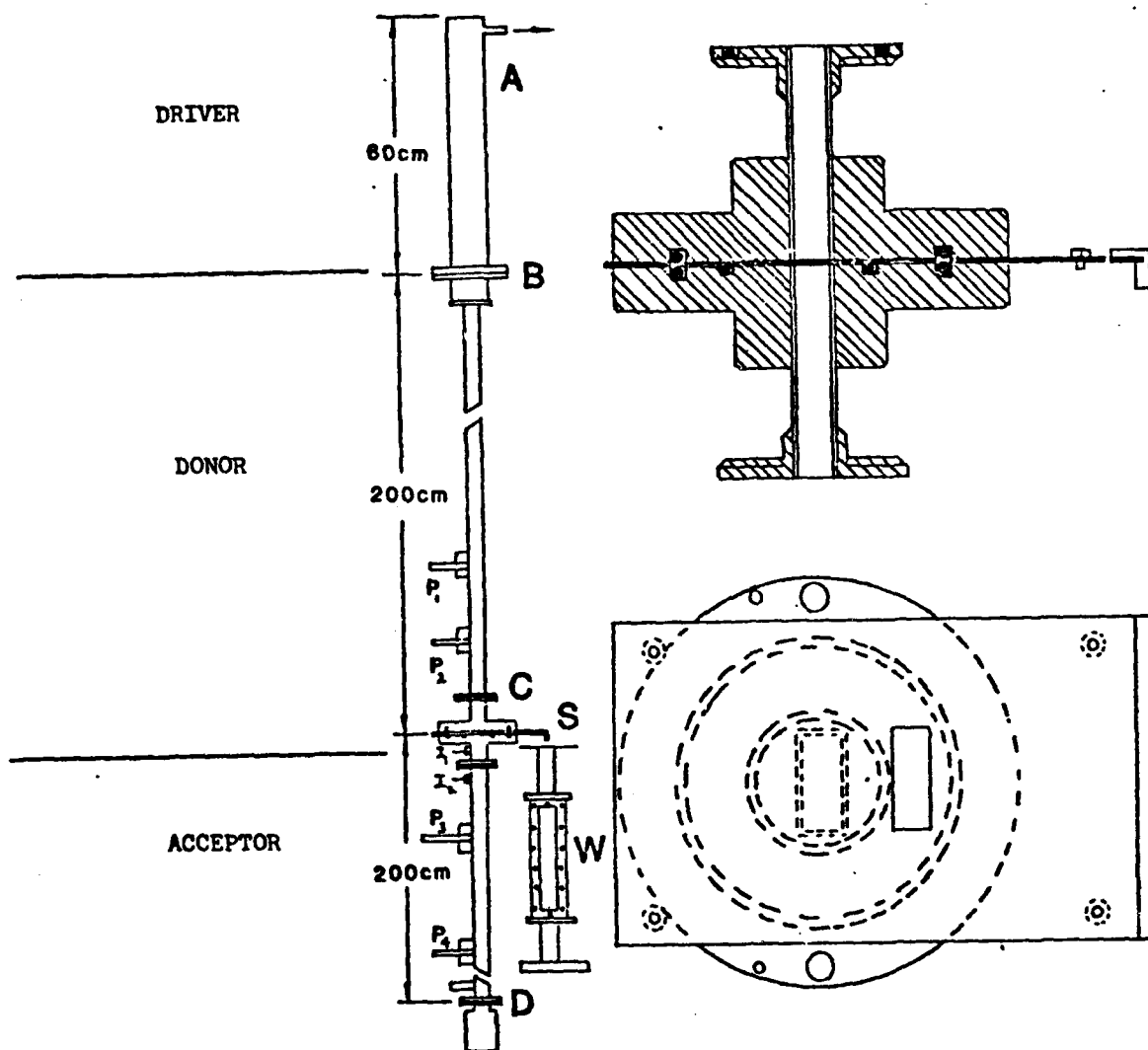


Figure 1. Detonation tube configuration used for interface studies. AB - Driver to ensure rapid establishment of a steady detonation in BC - the donor section. S - slide valve, SD - inert acceptor gas, W - optical window section for optical studies. For horizontal operation the detonation must be initiated within .25 sec. of the valve being opened to avoid buoyancy effects.

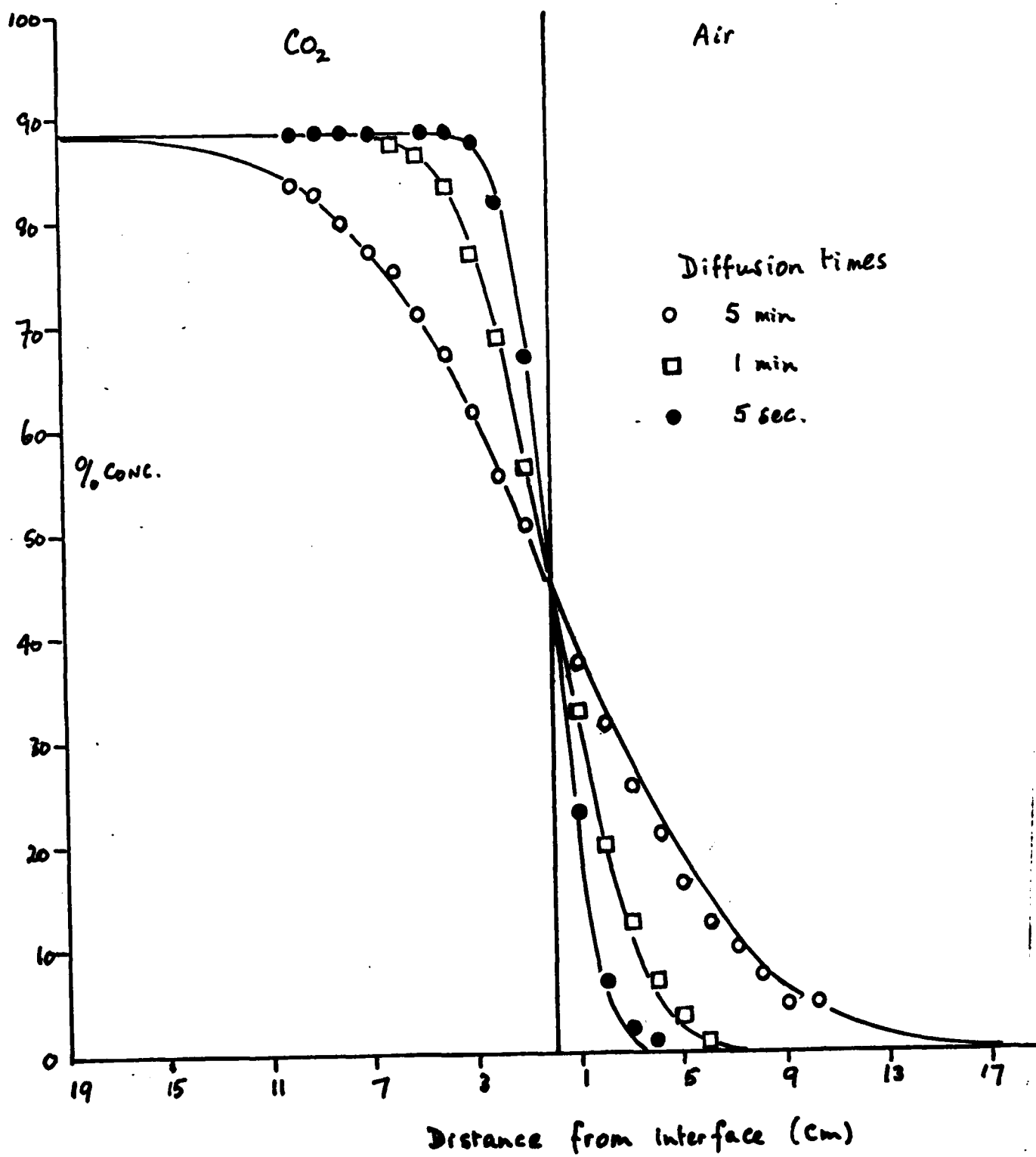
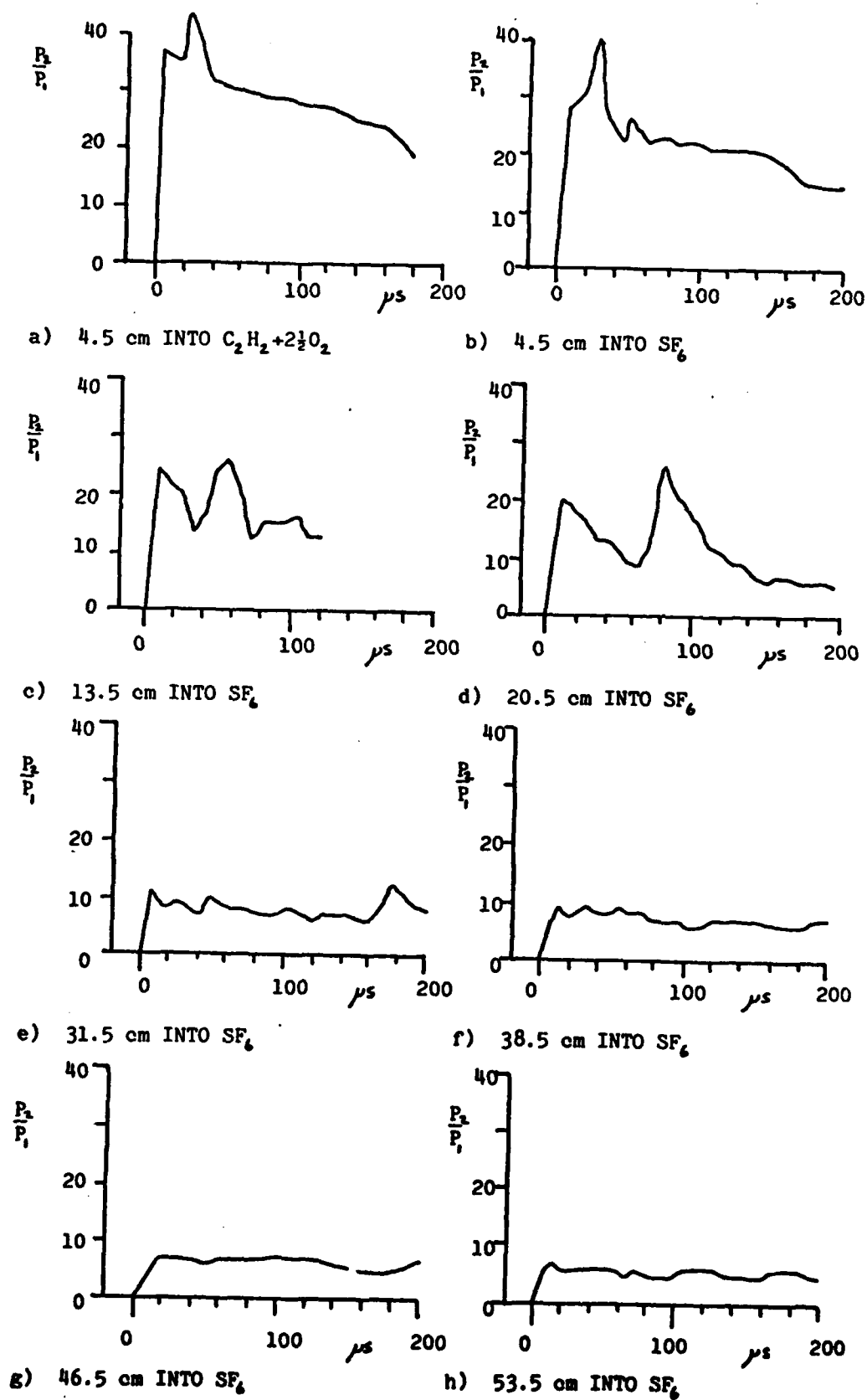


Figure 2



**Figure 3** PRESSURE PROFILES BEHIND A DETONATION IN  $C_2H_2 + 2\frac{1}{2}O_2$  TRAVELLING INTO  $SF_6$ . INITIAL PRESSURE 300 torr, DONOR LENGTH 1.25m.



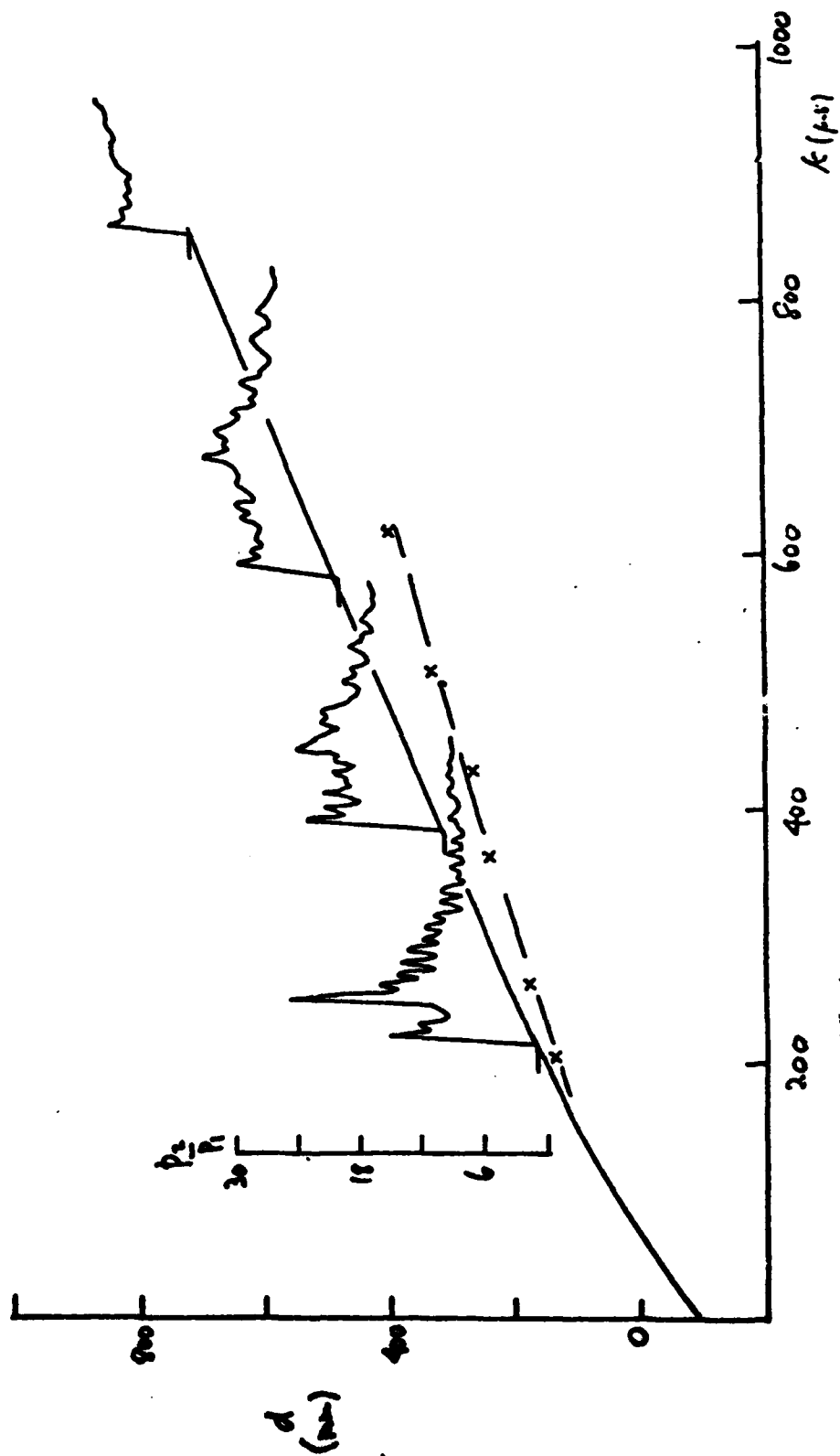


Figure 4  $C_2H_2 + 2.5O_2 / CO_2$  . Diffusion 2 min.

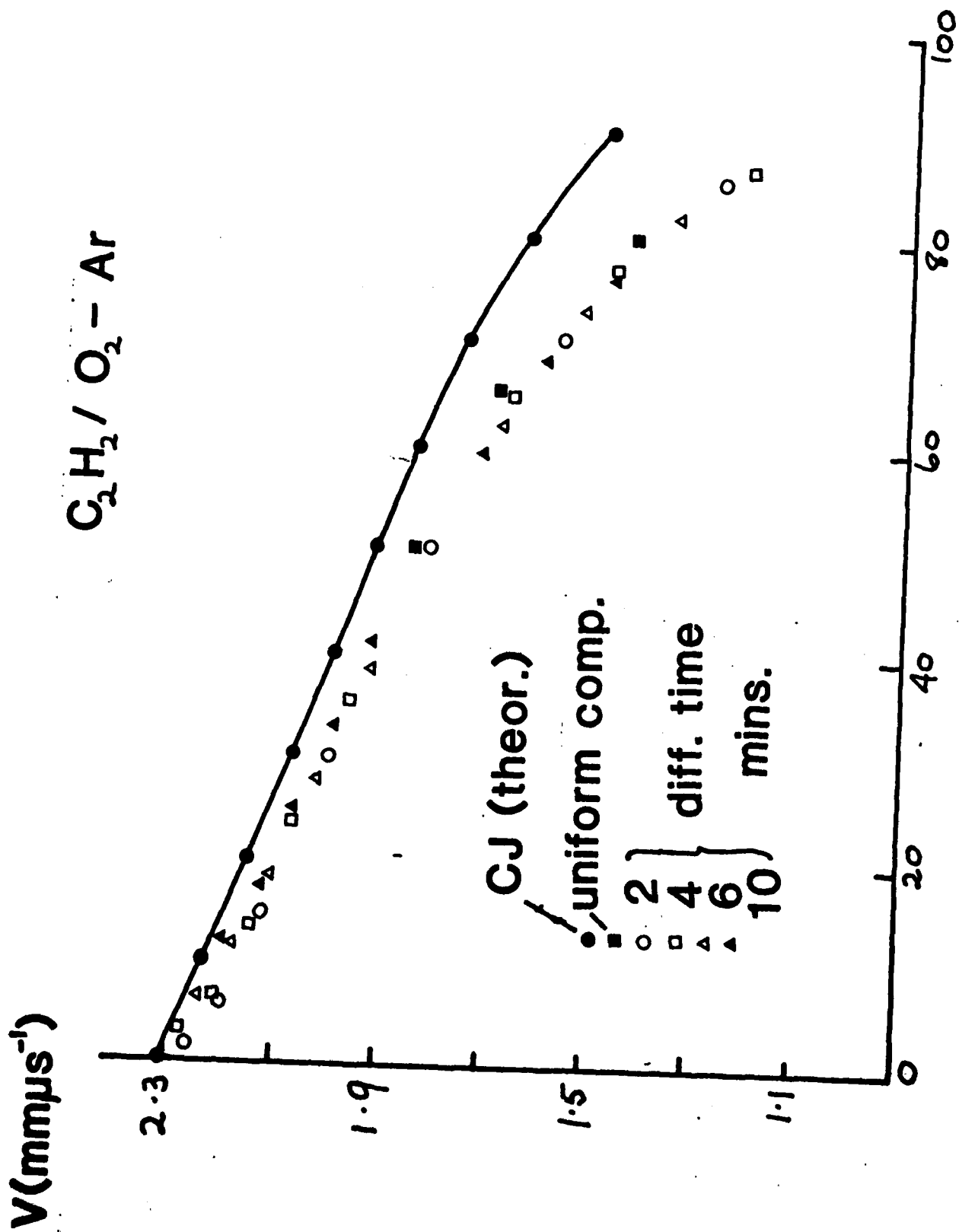


Figure 5

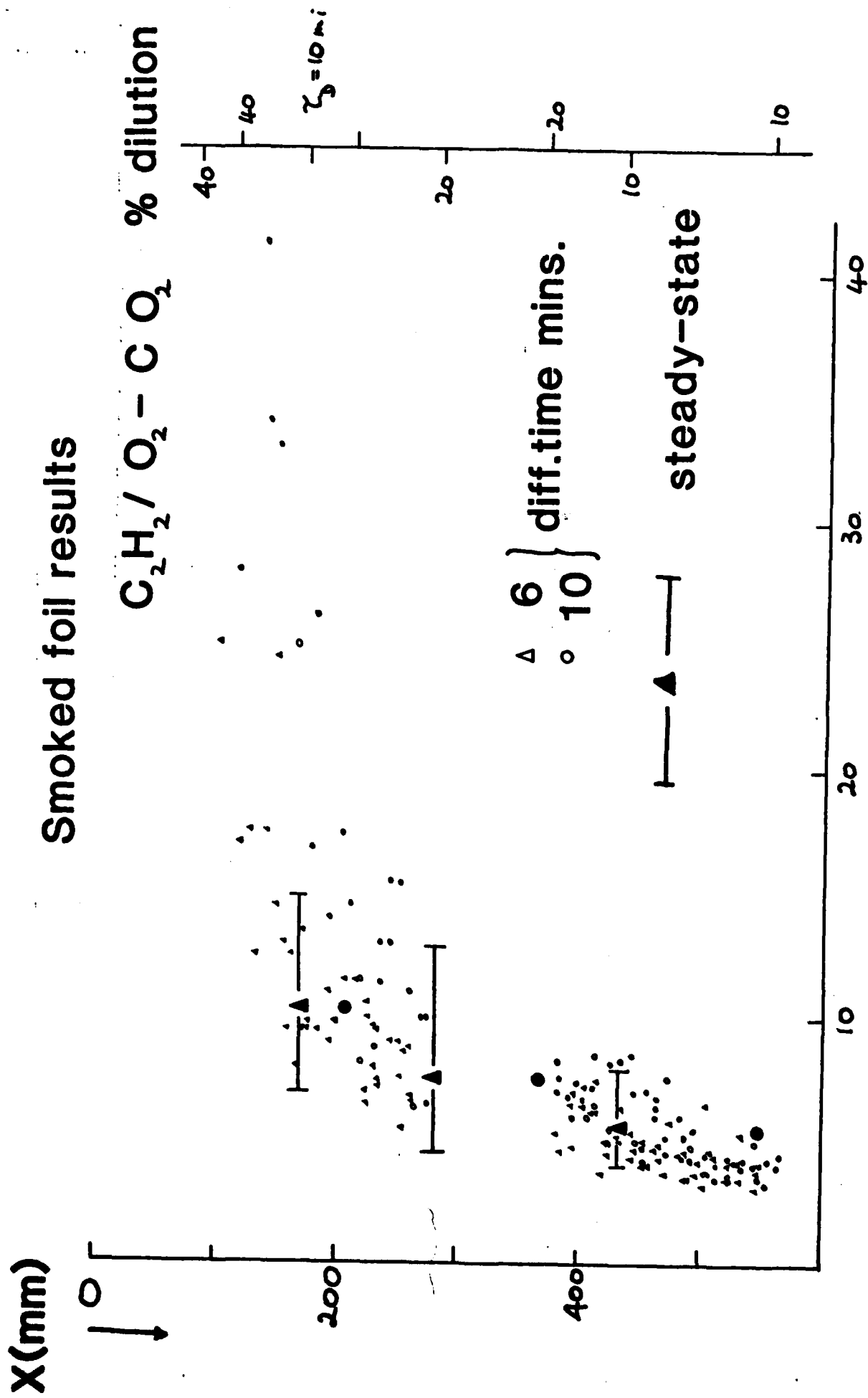


Figure 6 Cell length (mm)

X(mm)

$C_2H_2 / O_2 - Air$

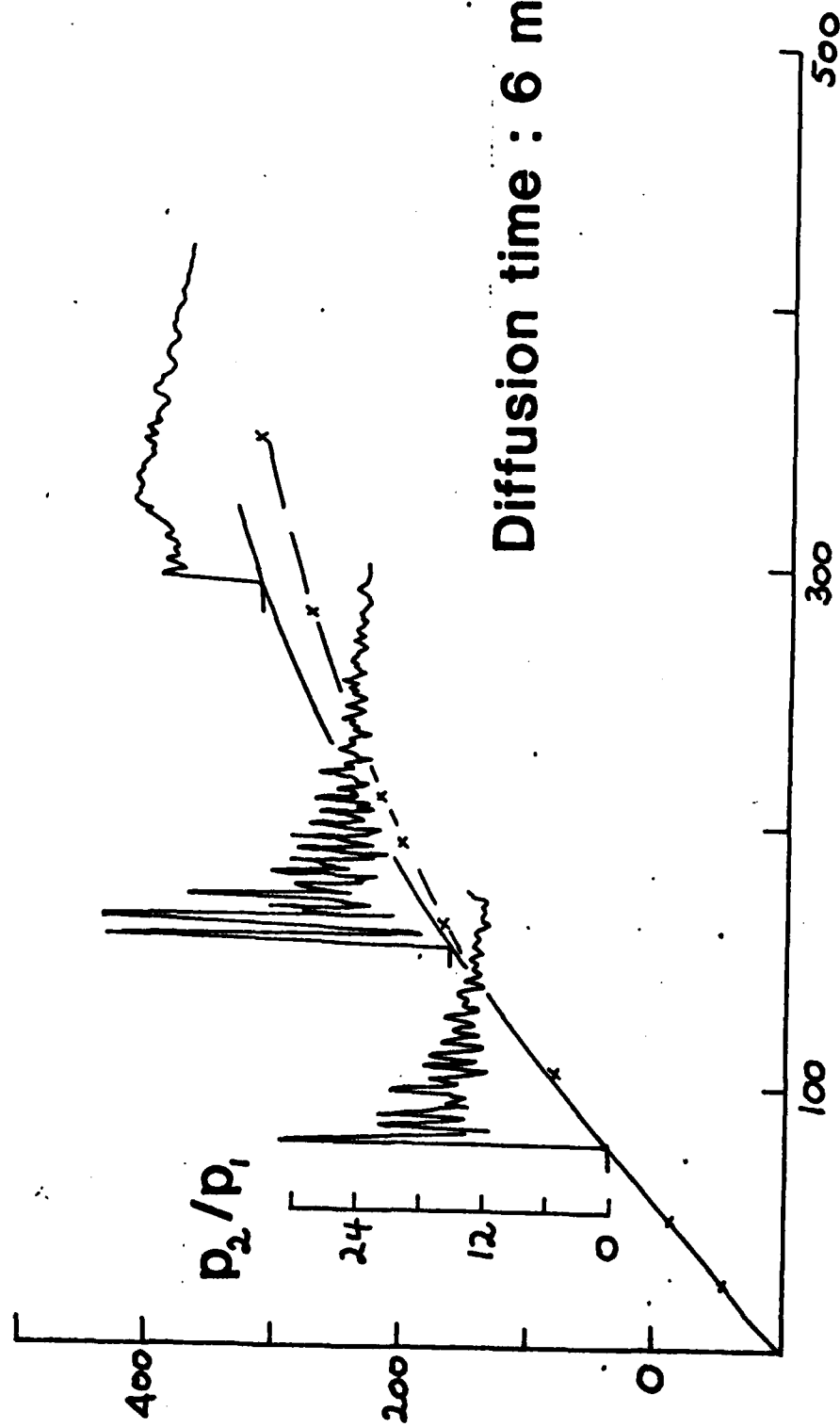
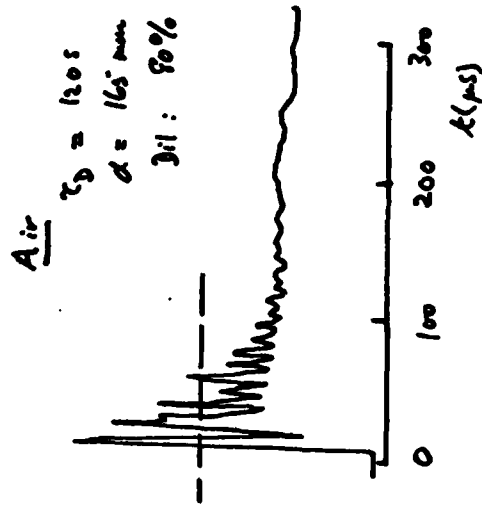
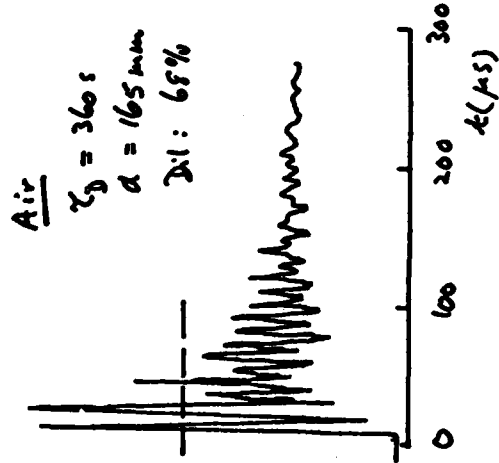
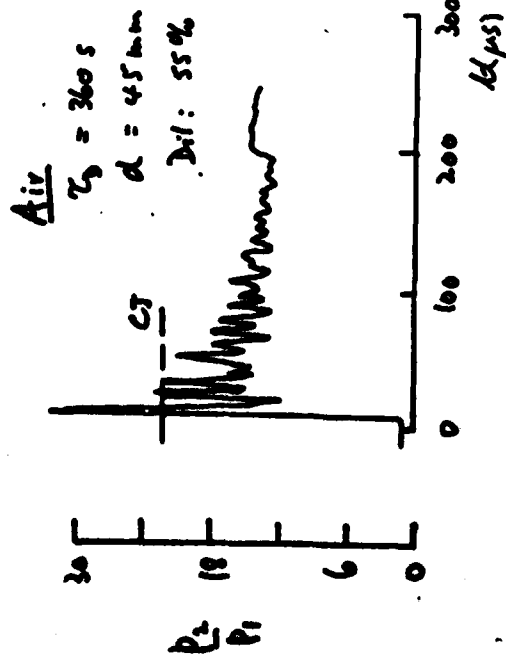
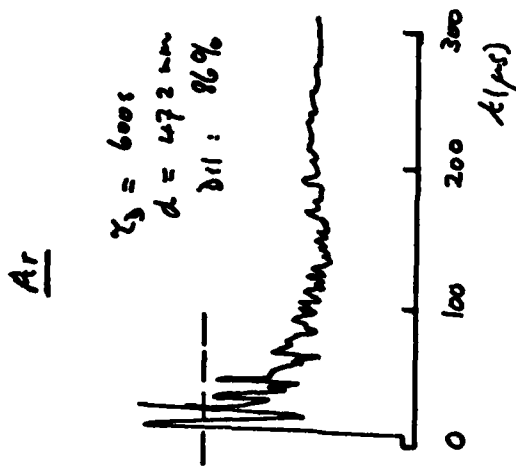
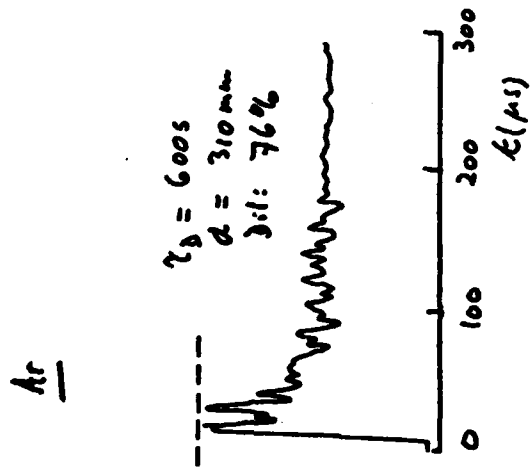
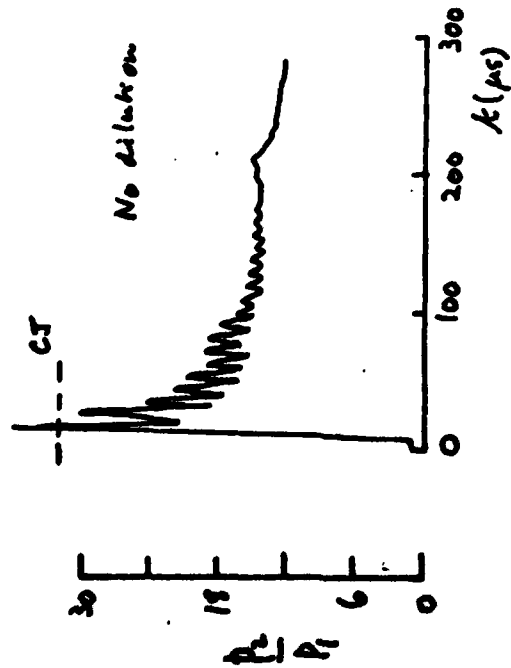


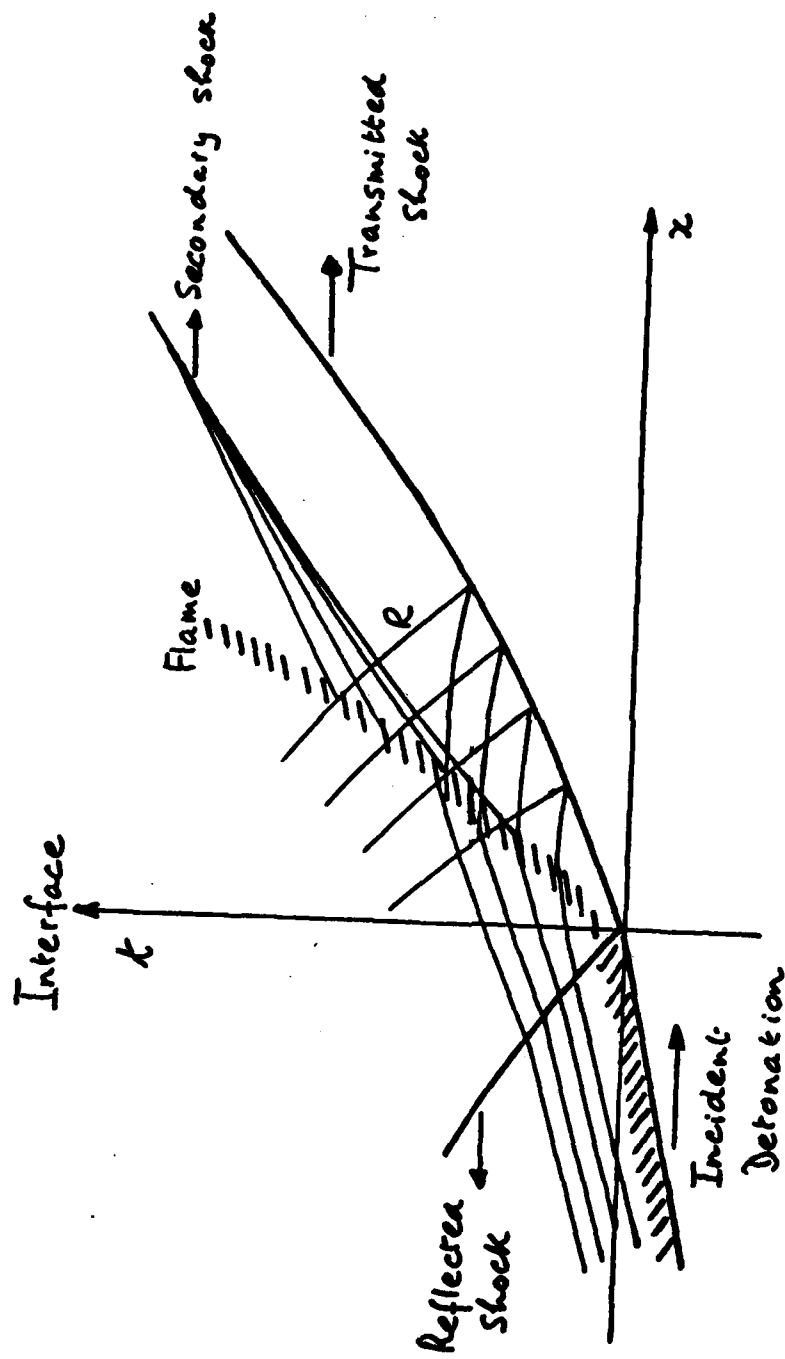
Figure 7

$t(\mu s)$



Static Pressure Profiles in Concentration gradients.  $\text{C}_2\text{H}_2 + 2.5\text{O}_2 / \text{Air} / \text{Ar}$ .  $P_1: 600\text{ Torr}$

Figure 8



Interaction of Detonation with steep concentration gradient

Figure 9

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